REMARKS

The applicant responds to the Office Action dated June 15, 2001, and overcomes each of the examiner's grounds for rejection of the claims.

All of the independent claims 1-3 have been amended and new dependent claims 4-18 have been added. According to an aspect of the invention, fixed bond information is derived. A delocalized representation of a chemical structure is analyzed. Based on valence information, a plurality of fixed bond representation candidates are identified for at least a portion of the chemical structure. At least a subset of the fixed bond representation candidates are evaluated. A selection is made from among the plurality of fixed bond representation candidates based on the evaluation.

Claim 1 has been rejected over Organic Chemistry, Third Edition, by Robert Thorton Morrison and Robert Neilson Boyd, copyright 1973 by Allyn and Bacon, Inc. ("the Organic Chemistry reference") and claims 1-3 have been rejected over U.S. Patent 5,461,580 to Facci et al. ("Facci") in view of the Organic Chemistry reference.

The Organic Chemistry reference is an organic chemistry textbook that discloses chemistry principles of valence and bonding.

Facci discloses an interactive chemical sketching system that deposits lines as the user traces with a mouse or other input device. The user determines the bond order. The Facci system can perform topological rotation of a feature about a ring. Facci discloses a library of templatized rings that allows a user to select a template and deposit a ring with few keystrokes or input events.

The Organic Chemistry reference and Facci are far removed from the pending claims. For example, all of the claims require analyzing a delocalized representation of a chemical structure and evaluating and selecting from among a plurality of fixed bond representation candidates for at least a portion of the chemical structure. The Organic Chemistry reference teaches nothing about analyzing a delocalized representation of a structure, much less also

evaluating and selecting from among a plurality of fixed bond representation candidates. The Organic Chemistry reference is concerned with bonding of atoms, and the physical meaning of both fixed and delocalized drawings, not analyzing, evaluating, and selecting different types of representations for the same chemical structure.

The Facci system provides no facility for analyzing a delocalized representation of a chemical structure and evaluating and selecting from among a plurality of fixed bond representation candidates for at least a portion of the chemical structure. There is no suggestion in Facci or the Organic Chemistry reference that the Facci system could be adapted to achieve such a facility. Facci's template library has chemically valid rings with respect to disposition of single and double bonds, for a few common ring sizes. For example, for a user who wants to sketch a six-membered ring, the library makes available a template with no double bonds, another template with one double bond, another template with two double bonds in a 1,3-relationship, another template with two double bonds in a 1,4-relationship, and another template with three double bonds. The user can invoke a bond-shifter function to rotate the bond pattern into proper place. However, the template library is a pre-computed, straightforward enumeration of a few valid all-carbon ring systems. The template library does not provide the Facci system with the ability to analyze a delocalized representation of a chemical structure and evaluate and select from among a plurality of fixed bond representation candidates for at least a portion of the chemical structure, as required by all the claims.

The dependent claims are patentable for at least the same reasons stated above.

The applicant submits that the application is in condition for allowance, which action is requested.

The Commissioner is hereby authorized to charge any fee deficiency, or credit any overpayment to our Deposit Account No. 08-0219.

Respectfully submitted,

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Replacement Pages for Claims 1-18

(MARKED TO SHOW CHANGES)

1. A method for use in deriving fixed bond information, comprising:

analyzing a delocalized representation of a chemical structure;

identifying [determining], based on valence information, [a table of electronic state and valence distributions, electronic and bonding characteristics for at least one atom in the chemical structure] a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

evaluating at least a subset of the fixed bond representation candidates; and

selecting from among the plurality of fixed bond representation candidates based on the evaluation [and

producing, based on the electronic and bonding characteristics, a fixed bond representation of the chemical structure].

2. A system for use in deriving fixed bond information, comprising:

an analyzer analyzing a delocalized representation of a chemical structure;

an identifier identifying [a determiner determining], based on valence information, [a table of electronic state and valence distributions, electronic and bonding characteristics for at least one atom in the chemical structure] a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

an evaluator evaluating at least a subset of the fixed bond representation candidates; and

a selector electing from among the plurality of fixed bond representation candidates based on the evaluation [and

a producer producing, based on the electronic and bonding characteristics, a fixed bond representation of the chemical structure].

3. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive fixed bond information, the instructions causing the system to:

analyze a delocalized representation of a chemical structure;

identify [determine], based on valence information, [a table of electronic state and valence distributions, electronic and bonding characteristics for at least one atom in the chemical structure] a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

evaluate at least a subset of the fixed bond representation candidates; and

select from among the plurality of fixed bond representation candidates based on the evaluation [and

produce, based on the electronic and bonding characteristics, a fixed bond representation of the chemical structure].

4. The method of claim 1, wherein at least a portion of the delocalized representation describes a monocyclic ring system.

5. The method of claim 1, wherein at least a portion of the delocalized representation describes a polycyclic ring system.

6. The method of claim 1, wherein at least a portion of the delocalized representation describes a ring system with a hetero substitution pattern.

7. The method of claim 1, wherein at least a portion of the delocalized representation describes a non-cyclic system.

8. The method of claim 1, wherein at least a portion of the delocalized representation describes an incompletely cyclic system.

9. The method of claim 1, further comprising:

including, in the produced fixed bond representation, a pair of opposite charges lacked by the delocalized representation.

10. The method of claim 1, further comprising:

including, in the produced fixed bond representation, a pair of radicals lacked by the delocalized representation.

11. The method of claim 1, further comprising:

queuing at least a subset of the candidates by priority.

12. The method of claim 1, further comprising:

using a precomputed table of atom valences as a function of element, charge, radical state, and number and distribution of bonds inside and outside of a delocalized region in the delocalized representation.

13. The method of claim 1, wherein the table includes an extensible component.

14. The method of claim 1, wherein the table is extensible to apply to any chemical element.

15. The method of claim 1, further comprising:

deriving electronic state and valence distributions information together with analyzing the delocalized representation.

16. The method of claim 1, further comprising:

determining whether it is practicable to produce a fixed bond representation of the chemical structure.

17. The method of claim 1, further comprising:

determining whether it is possible to produce a fixed bond representation of the chemical structure that meets a set of radicals requirements.

18. The method of claim 1, further comprising:

determining whether it is possible to produce a fixed bond representation of the chemical structure that meets a set of charges requirements.